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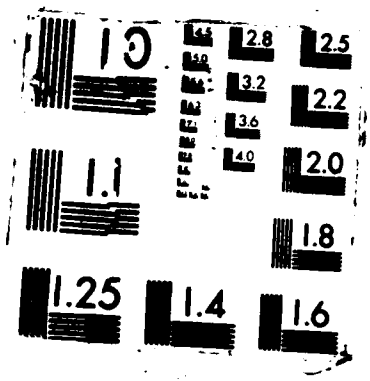
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Inhomogeneous Conditions at Open Boundaries for Wave Propagation Problems

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Inhomogeneous conditions at open boundaries for wave propagation problems

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Inhomogeneous conditions at open boundaries for wave propagation problems

1. Introduction

When wave propagation problems are solved numerically, it is often necessary to introduce artificial boundaries. In most cases no data are available at these boundaries, and therefore it is necessary to construct boundary conditions which in some way accounts for the behavior of the solution outside the computational domain Ω. Hence some assumption must be made which makes it possible to solve the problem exactly outside Ω, or alternatively to compute the solution approximately in a simple way. One such assumption is that the waves are propagating only in the outward direction across the boundary. This is the basis for various procedures in common use, the most general class being the absorbing boundary conditions, constructed by Engquist and Majda [1], [2], see also Higdon [7]. In [4] and [5] more general procedures were discussed, in particular the case with non-zero initial data outside the computational domain was considered.

The absorbing boundary conditions of higher order are formulated in terms of differentiated functions. As indicated in [4], this leads necessarily to weakly ill-posed problems, and as a consequence also to unstable numerical methods. This has been pointed out ~~and discussed by Higdon~~ [7] for the scalar wave-equation. The author argues that for conditions of order two or less, the possible effects of the instability is outweighed by the small reflection coefficients.

In this paper we ~~shall~~ investigate this problem further. When the initial data do not have compact support within the computational domain, or when some outside source is present, the boundary conditions become inhomogeneous. This tends to amplify the influence of the instability, and it becomes essential to modify the boundary procedure. We shall demonstrate how this can be done.

In Section 2 we treat the scalar wave equation, and we demonstrate the effect of higher order derivatives in the boundary conditions. More smoothness of the solution is required to compensate for the weak ill-posedness, and the approximation becomes more sensitive to perturbations. We also derive a stability estimate for the usual five-point approximation in one space dimension with the inhomogeneous version of the first absorbing boundary condition suggested in [1]. The estimate is an exact discrete version of the one obtained for the continuous problem.

In Section 3 we discuss general first order hyperbolic systems, and the implementation of higher order accurate boundary conditions. These are constructed such that the weak ill-posedness is removed, which makes it possible to construct stable approximations.

In a recent paper, Howell and Trefethen [8] have shown ill-posedness for migration equations in connection with certain boundary conditions. In this paper we consider the wave propagation problems in its original form, i.e., the differential equations are hyperbolic.

No attempt is made here to discuss various considerations concerning reflection properties. This has been done in the papers mentioned above. The purpose of this paper is only to illuminate the influence of the weak instabilities inherent with higher order derivatives in the boundary conditions, and how to remove them. These principles can also be applied to problems which are not of pure wave-propagation type.

2. The wave equation

We consider the wave equation where a scaling has been done such that the propagation speed is one. For convenience, we treat only the quarter-space problem

$$\begin{cases} \phi_{tt} = \phi_{xx} + \phi_{yy}\,, & 0 \le x < \infty,\ -\infty < y < \infty,\ 0 \le t, \\ \phi(x,0) = f(x,y)\,, \\ \phi_t(x,0) = d(x,y)\,, \end{cases} \tag{2.1}$$

where we need also a boundary condition at $x = 0$. The general theory for hyperbolic initial-boundary value problems is given in [9]. It is formulated for first order systems, but the same technique (the normal mode analysis) for analyzing well-posedness can be applied to differential equations and boundary conditions where higher order derivatives occur. We remark further on this in Section 3.

The problem is Laplace-transformed in the t-direction and Fourier-transformed in the y-direction, s and ω being the dual variables respectively. For $f = d = 0$, the transformed solution to (2.1) is

$$\hat{\phi}(x,\omega,s) = e^{-x\sqrt{s^2+\omega^2}}\,\hat{\phi}(0,\omega,s)\,,$$

where the square root is defined such that $\mathrm{Re}\,\sqrt{z} \ge 0$ for all z. If the transformed boundary condition is

$$\hat{B}(\omega,s)\hat{\phi}(0,\omega,s) = \hat{g}(\omega,s)\,,$$

the *uniform Kreiss condition* required for well-posedness is

$$|\hat{B}(\omega,s)| \ge \delta > 0\,, \quad \mathrm{Re}\,s \ge 0,\ \ \mathrm{Im}\,\omega = 0\,. \tag{2.2}$$

When the wave function ϕ is specified at $x = 0$, such that

$$\phi(0,y,t) = g(y,t)\,, \tag{2.3}$$

we have $\hat{B} = 1$, and the condition (2.2) is trivially satisfied.

Consider next the boundary condition

$$\phi_t - \phi_x = g(y,t)\,, \quad x = 0\,, \tag{2.4}$$

which is the inhomogeneous version of the first absorbing boundary condition. The problem of providing the data $g(y,t)$ will be discussed in Section 3. For (2.4) we have

$$\hat{B}(\omega,s) = s + \sqrt{s^2+\omega^2}\,,$$

and obviously the condition (2.2) is violated for $\omega = s = 0$. When the Kreiss condition is violated for $s = s_0$ on the imaginary axis, s_0 is called a generalized eigenvalue. In such a case the problem is said to be weakly ill-posed. However, it seems natural to accept first order derivatives in the boundary conditions when the differential equation is of second order, and we shall further investigate this case.

Since the generalized eigenvalue occurs for $\omega = 0$, it is sufficient to study the one-dimensional case. We consider the problem

$$
\text{(2.5)} \qquad \begin{cases} \text{(a)} & \phi_{tt} = \phi_{xx}\,, & 0 \le x < \infty,\ 0 \le t \\ \text{(b)} & \phi_t - \phi_x = g(t)\,, & x = 0 \\ \text{(c)} & \phi = f(x)\,, & t = 0 \\ \text{(d)} & \phi_t = d(x)\,, & t = 0. \end{cases}
$$

It is assumed that f, d have compact support, such that for any given t, $\phi(x,t)$ also has compact support. The solution of (2.5) can be given explicitly, but we derive the general estimate for the solution in order to get a procedure that can be modified in a straightforward manner to discretizations of (2.5).

The wave equation is rewritten as a first order system. With

$$
u = \phi_t\,, \quad v = \phi_x
$$

we get

$$
\begin{cases} \begin{bmatrix} u \\ v \end{bmatrix}_t = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}_x, & 0 \le x < \infty,\ 0 \le t \\ u - v = g(t)\,, & x = 0 \\ u = d(x)\,, & t = 0 \\ v = f'(x)\,, & t = 0. \end{cases}
$$

Since the ingoing characteristic variable is prescribed, we get an estimate also for the boundary values of the solution. A straightforward application of the energy method gives

$$
\begin{aligned} &\|u(t)\|^2 + \|v(t)\|^2 + \int_0^t (|u(0,\tau)|^2 + |v(0,\tau)|^2)\,d\tau \\ &\qquad \le C\left(\|d\|^2 + \|f'\|^2 + \int_0^t |g(\tau)|^2\,d\tau\right) \end{aligned} \qquad \text{(2.6)}
$$

where $\|\cdot\|$ denotes the L_2-norm. Note that the reformulation as a first order system has eliminated the generalized eigenvalue $s = 0$, making the estimate (2.6) possible.

In order to get an estimate also for ϕ, we use the fact that $\phi(x,t)$ has compact support, and obtain for some $x_0 = x_0(t)$,

$$
\|\phi(t)\|^2 = \int_0^{x_0} \left[\int_0^x v(\xi,t)\,d\xi + \phi(0,t)\right]^2 dx \le C(\|v(t)\|^2 + |\phi(0,t)|^2)\,,
$$

$$
|\phi(0,t)|^2 = |f(0) + \int_0^t u(0,\tau)\,d\tau|^2 \le 2\left(|f(0)|^2 + \int_0^t |u(0,\tau)|^2\,d\tau\right). \qquad \text{(2.7)}
$$

The integral in the right hand side of (2.7) can be estimated by using (2.6), and we arrive at the final estimate

$$
\begin{aligned} &\|\phi(t)\|^2 + \|\phi_t(t)\|^2 + \|\phi_x(t)\|^2 + |\phi(0,t)|^2 + \int_0^t (|\phi_t(0,\tau)|^2 + |\phi_x(0,\tau)|^2)\,d\tau \\ &\qquad \le C\left(\|d\|^2 + \|f'\|^2 + |f(0)|^2 + \int_0^t |g(\tau)|^2\,d\tau\right), \end{aligned} \qquad \text{(2.8)}
$$

where C depends on t. Here the derivatives of ϕ and of the initial data are included, which is very natural. These derivatives are physical quantities of prime interest, and (2.8) is therefore a useful estimate. For non-smooth initial data an estimate can still be obtained. With the variable substitution

$$u = \phi$$

$$v = \int_0^t \phi_x(x,\tau)\,d\tau + \int_0^x d(\xi)\,d\xi$$

we get after integrating (2.5b) with respect to t,

$$\begin{cases} \begin{bmatrix} u \\ v \end{bmatrix}_t = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}_x, & 0 \le x < \infty,\ 0 \le t \\ u - v = \tilde{g}(t), & x = 0 \\ u = f(x), & t = 0 \\ v = \int_0^x d(\xi)\,d\xi, & t = 0, \end{cases}$$

where

$$\tilde{g}(t) = \int_0^t g(\tau)\,d\tau + f(0).$$

Corresponding to (2.6) we get

$$\|\phi(t)\|^2 + \int_0^t |\phi(0,\tau)|^2\,d\tau \le C\left(\|f\|^2 + \|\int_0^x d(\xi)\,d\xi\|^2 + \int_0^t |\tilde{g}(\tau)|^2\,d\tau\right)$$

Next, consider the boundary condition

$$\phi_{tt} - \phi_{xt} - \tfrac{1}{2}\phi_{yy} = g(y,t). \tag{2.9}$$

For $g(y,t) = 0$, this is the second absorbing boundary condition. In transformed space, the Kreiss condition obtained from (2.9) is

$$\hat{B}(\omega,s) \equiv s(s + \sqrt{s^2+\omega^2}) + \tfrac{1}{2}\omega^2 \neq 0, \qquad \text{Re } s \ge 0. \tag{2.10}$$

For $\omega = 0$, $s = 0$, the condition is not fulfilled, and we again have a generalized eigenvalue. (This case was not included in the analysis carried out in [1], [2], and [10].)

In the analysis of the one-dimensional problem above, the final estimate was obtained by considering a first order system for the derivatives of ϕ. For the higher order boundary condition, we apply the same technique once more. The functions $\tilde{u} = \phi_{tt}$, $\tilde{v} = \phi_{xt}$ satisfy the same differential equation as u, v above, but with new initial conditions, which can be derived by using the differential equation. We get

$$\begin{cases} \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}_t = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}_x, & 0 \le x < \infty,\ 0 \le t \\ \tilde{u} - \tilde{v} = g(t), & x = 0 \\ \tilde{u} = f''(x), & t = 0 \\ \tilde{v} = d'(x), & t = 0. \end{cases}$$

Corresponding to (2.6) we obtain the estimate

$$\|\tilde{u}(t)\|^2 + \|\tilde{v}(t)\|^2 + \int_0^t (|\tilde{u}(0,\tau)|^2 + |\tilde{v}(0,\tau)|^2)\, d\tau \le C \left(\|f''\|^2 + \|d'\|^2 + \int_0^t |g(\tau)|^2\, d\tau \right).$$

By going back to ϕ via u, v, we can obtain an estimate for ϕ, but now in terms of higher order derivatives.

As we demonstrated above, the introduction of higher derivatives in the estimates can be avoided by integrating the boundary condition with respect to time. The analogous technique can in general not be applied for difference approximations. Furthermore, perturbations in derivative boundary conditions produce a possible polynomial growth in time, which propagates into the domain. For approximations there will be a growth of the solution which is at least proportional to n. For each extra factor s that multiplies the function $\hat{B}(\omega, s)$ in (2.2), the possible polynomial growth in the approximation increases one order in n. In general, one should therefore avoid derivative boundary conditions, for first order systems.

In order to make these conjectures more precise, we consider difference approximations to the wave equation. Our approach is to use a technique similar to the one for the continuous case, in order to obtain estimates of the solution. We treat only the standard 5-point formula, and consider first the Cauchy-problem

$$\text{(2.11)} \qquad \begin{cases} \phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1} = \lambda^2(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n), \quad \lambda = k/h \\ \phi_j^0 = f_j \\ \phi_j^1 = f_j + k d_j, \end{cases}$$

where k, h are the time- and space-steps respectively. (Other initial procedures could of course be used, but this one is enough for our purposes.) After Fourier-transformation in x, we get

$$\hat{\phi}_\omega^{n+1} - 2\left(1 - 2\lambda^2 \sin^2 \tfrac{\omega h}{2}\right) \hat{\phi}_\omega^n + \hat{\phi}_\omega^{n-1} = 0,$$

which has the characteristic roots z_1, z_2 on the unit circle if $\lambda \le 1$. For $\omega = 0$ they coincide at $z = 1$; accordingly there is a possible growth in the solution of order n. This cannot be avoided with any consistent method. By choosing the initial data such that $u_j^1 - u_j^0 = O(k)$ (corresponding to a bounded d-function in (2.11)), the growth is at most of order $t_n = nk$, which is the same as for the differential equation. But one should be aware of the fact that perturbations in the initial data are magnified, and that the scalar wave equation is not suitable for integration over very long time intervals.

We next introduce discrete boundary conditions. We shall use the difference operators

$$\Delta_{\pm x}\phi_j^n = hD_{\pm x}\phi_j^n = \pm(\phi_{j\pm1}^n - \phi_j^n)$$
$$\Delta_{\pm t}\phi_j^n = kD_{\pm t}\phi_j^n = \pm(\phi_j^{n\pm1} - \phi_j^n).$$

The inhomogeneous version of the first condition used in [1] which approximates the boundary condition in (2.5) is

$$\text{(2.12)} \qquad D_{+t}(\phi_0^n + \phi_1^n) - D_{+x}(\phi_0^n + \phi_0^{n+1}) = 2g(t_{n+1/2}).$$

In order to obtain correct centering, the grid is shifted such that $x_0 = -h/2$. By introducing the new variables

$$u_j^{n+1} = D_{-t}\phi_j^{n+1},$$
$$v_j^n = D_{+x}\phi_j^n,$$

the difference scheme can be written in the form

$$\text{(2.13)} \qquad \begin{cases} \text{(a)} & u_j^{n+1} - u_j^n = \lambda \Delta_{-x} v_j^n, & j = 1, 2, \dots \\ \text{(b)} & v_j^{n+1} - v_j^n = \lambda \Delta_{+x} u_j^{n+1}, & j = 0, 1, \dots \\ \text{(c)} & u_j^1 = d_j, & j = 0, 1, \dots \\ \text{(d)} & v_j^0 = D_{+x} f_j, & j = 0, 1, \dots . \end{cases}$$

The boundary condition (2.12) is

$$\text{(2.14)} \qquad u_1^{n+1} + u_0^{n+1} - (v_0^{n+1} + v_0^n) = 2g(t_{n+1/2}).$$

From now on, the notation $\|\cdot\|$ is used for the discrete l_2-norm defined by

$$\text{(2.15)} \qquad \|u^n\|^2 = \sum_{j=0}^{\infty} |u_j^n|^2 h.$$

We shall prove

Theorem 2.1. *The boundary condition (2.14) gives a stable difference scheme (2.13) for $\lambda < 1$, and for $0 \le t_n \le T$ there is an estimate*

$$\text{(2.16)} \qquad \|u^n\|^2 + \|v^n\|^2 + \sum_{\nu=1}^{n} (|u_0^\nu|^2 + |v_0^\nu|^2) k \le C \left(\|d\|^2 + \|D_{+x} f\|^2 + \sum_{\nu=1}^{n} |g(t_{\nu-1/2})|^2 k \right).$$

Proof. The normal mode analysis, see [6], is applied. We need the general form of the solution to the transformed system

$$(z-1)\hat{u}_j = \lambda(\hat{v}_j - \hat{v}_{j-1}), \qquad j = 1, 2, \dots$$
$$(z-1)\hat{v}_j = \lambda z(\hat{u}_{j+1} - \hat{u}_j), \qquad j = 0, 1, \dots .$$

When requiring bounded solutions for $|z| > 1$, there is only one component present, and it has the form

$$\text{(2.17)} \qquad \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix}_j = \sigma \begin{bmatrix} 1 \\ \pm\kappa\sqrt{z/\kappa} \end{bmatrix} \kappa^j.$$

Here the constant σ is determined by the boundary condition, and κ satisfies the characteristic equation

$$\text{(2.18)} \qquad (z-1)^2 = \lambda^2 \frac{z}{\kappa} (\kappa - 1)^2$$

i.e., we have

$$z - 1 = \pm\lambda \sqrt{\frac{z}{\kappa}}\,(\kappa - 1)\,. \tag{2.19}$$

The upper and lower signs in (2.17) and (2.19) correspond to each other, and are chosen such that $|\kappa| < 1$ for $|z| > 1$.

The transformed boundary condition (2.14) is

$$z(\hat{u}_1 + \hat{u}_0) - (z+1)\,\hat{v}_0 = 2\hat{g}$$

and when (2.17) is inserted, we get for $\hat{g} = 0$,

$$z + 1 = \pm\frac{z}{\kappa} \sqrt{\frac{\kappa}{z}}\,(\kappa + 1)\,. \tag{2.20}$$

We shall prove that there is no solution z, κ to (2.19), (2.20) with $|z| \geq 1$. By squaring both sides of (2.20) we get

$$z^2 - \left(\kappa + \tfrac{1}{\kappa}\right)\, z + 1 = 0\,.$$

Obviously the coefficient of z in this equation must equal the coefficient of z in (2.18), i.e.,

$$\kappa + \tfrac{1}{\kappa} = 2(1 - \lambda^2) + \lambda^2 \left(\kappa + \tfrac{1}{\kappa}\right)\,,$$

and this is possible for $\lambda < 1$ only if $\kappa = 1$. This corresponds to $z = 1$ in (2.19), and a perturbation $z = 1 + \delta$, $\delta > 0$ shows that the corresponding root κ is inside the unit circle if the lower sign is chosen. But in that case (2.20) does not hold, showing that the Kreiss condition is fulfilled.

The norm used in [6] is integrated in time, furthermore there is an assumption of zero initial data. However, if the approximation fulfills an energy-estimate for periodic solutions, then the l_2-norm of the solution can be estimated at any given time in terms of the initial and boundary data. That part of the proof is omitted here, we refer to [3] for the proof in the semi-discrete case.

The energy estimate for periodic boundary conditions is easily obtained. Define the scalar product and norm for scalar periodic grid-functions by

$$(u, v)_p = \sum_{j=1}^{N} u_j v_j h\,, \qquad \|u\|_p^2 = (u, u)_p$$

where $u_j = u_{j+N}$. By taking the scalar product of (2.13a) with u^{n+1}, and of (2.13b) with v^{n+1}, we get

$$\|u^{n+1}\|_p^2 = (u^n, u^{n+1})_p + \lambda(\Delta_{-x} v^n, u^{n+1})_p$$
$$\|v^{n+1}\|_p^2 = (v^n, v^{n+1})_p + \lambda(\Delta_{+x} u^{n+1}, v^{n+1})_p\,.$$

From (2.13a), (2.13b) we also get

$$(u^n, u^{n+1})_p = \|u^n\|_p^2 + \lambda(\Delta_{-x} v^n, u^n)_p$$
$$(v^{n+1}, v^n)_p = \|v^n\|_p^2 + \lambda(\Delta_{+x} u^{n+1}, v^n)_p\,,$$

and by using the identity

$$(\Delta_{-x}v, u)_p = -(\Delta_{+x}u, v)_p$$

we obtain

$$E(U^{n+1}) = E(U^n)\,, \tag{2.21}$$

where

$$E(U^n) = \|u^n\|_p^2 + \|v^n\|_p^2 + \lambda(\Delta_{-x}v^n, u^n)_p\,.$$

Since

$$|(\Delta_{-x}v, u)_p| \le \|v\|_p^2 + \|u\|_p^2\,,$$

$E(U^n)$ is a proper energy-norm, which for $\lambda < 1$ is equivalent to $\|u^n\|_p^2 + \|v^n\|_p^2$. This proves the theorem.

By using the definition of u and v we get immediately from Theorem 2.1:

Corollary 2.1. *The solution to the discrete wave equation (2.11) with boundary condition (2.12) satisfies the estimate*

$$\|\phi^n\|^2 + \|D_{-t}\phi^n\|^2 + \|D_{+x}\phi^n\| + |\phi_0^n|^2 + \sum_{\nu=1}^{n}(|D_{-t}\phi_0^\nu|^2 + |D_{+x}\phi_0^n|^2)k$$
$$\le C\left(\|d\|^2 + \|D_{+x}f\|^2 + |f_0|^2 + \sum_{\nu=1}^{n}|g(t_{\nu-1/2})|^2 k\right)\,.$$

This inequality corresponds exactly to the corresponding one (2.8) for the continuous case.

Next we shall consider the higher order boundary condition (2.9) for the one-dimensional scheme. The approximation used in [1] for this condition is

$$D_{+t}D_{-t}(\phi_0^n + \phi_1^n) - \tfrac{1}{k}\,D_{+x}(\phi_0^{n+1} - \phi_0^{n-1}) = 2g(t_n)\,,$$

which stated in terms of the variables u, v takes the form

$$u_0^{n+1} - u_0^n + u_1^{n+1} - u_1^n - (v_0^{n+1} - v_0^{n-1}) = 2kg(t_n)\,. \tag{2.22}$$

The stability analysis follows the same lines as for the first order condition. In fact, the proof of Theorem 2.1 is identical up to the condition (2.20), which for (2.22) becomes

$$(z-1)[z + 1 \mp \frac{z}{\kappa}\sqrt{\frac{z}{\kappa}}(\kappa+1)] = 0\,. \tag{2.23}$$

The extra factor $z - 1$ is a result of the time-differentiation applied on the boundary condition. Since (2.23) holds for $z = 1$ regardless of the sign in the brackets, there is necessarily a generalized eigenvalue $z = 1$ corresponding to $\kappa = 1$. Therefore the scheme is unstable, and small perturbations in the difference scheme or the boundary conditions can be expected to have a significant effect on the solution.

We shall further investigate the approximation in order to see if it is possible to obtain estimates under more restrictive smoothness assumptions. This will explain why under certain circumstances higher order absorbing boundary conditions can be used. We use the same technique as indicated for the continuous problem. Corresponding to the differentiated variables u_t, v_t we define

$$\tilde{u}_j^{n+1} = D_{-t} u_j^{n+1}, \qquad j = 0, 1, \ldots; \; n = 1, 2, \ldots$$
$$\tilde{v}_j^{n+1} = D_{-t} v_j^{n+1}, \qquad j = 0, 1, \ldots; \; n = 0, 1, \ldots.$$

By differencing the system (2.13) in the time-direction, we get

$$\text{(2.24)} \qquad \begin{cases} \tilde{u}_j^{n+1} - \tilde{u}_j^n = \lambda \Delta_{-x} \tilde{v}_j^n, & j = 1, 2, \ldots; \; n = 2, 3, \ldots \\ \tilde{v}_j^{n+1} - \tilde{v}_j^n = \lambda \Delta_{+x} \tilde{u}_j^{n+1}, & j = 0, 1, \ldots; \; n = 1, 2, \ldots \\ \tilde{u}_j^2 = \frac{1}{k^2} (\phi_j^2 - 2\phi_j^1 + \phi_j^0), & j = 0, 1, \ldots \\ \tilde{v}_j^1 = \frac{1}{kh} (\phi_{j+1}^1 - \phi_j^1 - \phi_{j+1}^0 + \phi_j^0), & j = 0, 1, \ldots. \end{cases}$$

The boundary condition (2.22) takes the form

$$\tilde{u}_0^{n+1} + \tilde{u}_1^{n+1} - (\tilde{v}_0^{n+1} + \tilde{v}_0^n) = 2g(t_n).$$

Apparently $\tilde{u}^n$, $\tilde{v}^n$ satisfy the same difference equation and the same type of boundary conditions as the solution (u^n, v^n) to (2.13), (2.14) does. Therefore, an estimate of the type (2.16) holds. However, in this case the initial data $\tilde{u}^2$, $\tilde{v}^1$ as given in (2.24) are different, and this is an important distinction. Even if the grid-function ϕ is bounded, it cannot be expected to be smooth unless we are very careful when initializing the problem. In particular, it may be difficult to match the initial data to the boundary data. If this is not done properly, accuracy will be lost. (In [1] the need for compatible boundary and initial data is pointed out, but the connection to stability and accuracy is not discussed.)

As an example, consider a case where $\phi(x, t) \equiv 0$ for $t \leq 0$, and where a boundary function $g(t)$ begins driving the solution at $t = 0$, i.e., $g(t) = 0$ for $t \leq 0$. We compare the boundary condition

$$\text{(2.25)} \qquad \phi_t - \phi_x = g(t), \quad x = 0$$

with its differentiated version

$$\phi_{tt} - \phi_{xt} = g'(t), \qquad x = 0,$$

corresponding to the first and second order conditions (2.4) and (2.9) respectively. For convenience we extend the grid one step backwards in time, such that the initial conditions are

$$\phi_j^{-1} = \phi_j^0 = 0, \qquad j = 0, 1, \ldots.$$

The discrete first order boundary condition is (2.12). We use the first order system (2.13) to compute the first points. It turns out that $\lambda = 1$ gives the best local accuracy near $x = 0$, $t = 0$, and a direct calculation shows that with (2.13), (2.14), we get

$$u_1^2 = g(k/2) = g(0) + \tfrac{k}{2} g'(0) + O(k^2).$$

Since the left-going wave $u+v$ is zero, the true solution is $u(x,t) = 0.5g(t-x)$ for $x \le t$. Recalling that u_j^n is centered at $(x_j, t_{n-1/2})$, the true solution corresponding to u_1^2 is

$$u(k/2, 3k/2) = 0.5g(k) = 0.5[g(0) + kg'(0) + O(k^2)] .$$

Apparently a second order error is obtained only if

$$g(0) = 0 .$$

The second order boundary condition is

$$u_0^{n+1} - u_0^n + u_1^{n+1} - u_1^n - (v_0^{n+1} - v_0^{n-1}) = 2kg'(t_n) .$$

In this case we get for $\lambda = 1$,

$$u_1^2 = kg'(0)$$

which is accurate to order k^2 only if

$$g(0) = g'(0) = 0 .$$

The conclusion is that if $g'(0) \neq 0$, the approximation becomes *worse* with the higher order boundary condition. Both boundary conditions are centered properly, so this is an illustration of the fact that higher order derivatives in the boundary conditions require smoother solutions. Convergence may still occur as $h \to 0$, which was demonstrated for a scalar equation in [5], but in general accuracy is lost.

A simple numerical experiment was performed in order to illustrate the results obtained above. We used the interval $0 \le x \le 1$, and the right boundary was treated similarly to the left one, but with zero data. With zero initial data $f(x)$, $d(x)$, the solution is generated by the boundary data $g(t)$ in (2.5), and the true solution $\phi(x,t)$ is easily derived.

The three alternative boundary conditions are

$$\text{BC0} \quad \begin{cases} \phi_0^n = \phi(-h/2, t_n) \\ \phi_{N+1}^n = \phi(1 + h/2, t_n) \end{cases}$$

$$\text{BC1} \quad \begin{cases} \Delta_{+t}(\phi_0^n + \phi_1^n) - \lambda \Delta_{+x}(\phi_0^n + \phi_0^{n+1}) = 2kg(t_{n+1/2}) \\ \Delta_{+t}(\phi_N^n + \phi_{N+1}^n) + \lambda \Delta_{+x}(\phi_N^n + \phi_N^{n+1}) = 0 \end{cases}$$

$$\text{BC2} \quad \begin{cases} \Delta_{+t}\Delta_{-t}(\phi_0^n + \phi_1^n) - \lambda \Delta_{+x}(\phi_0^{n+1} - \phi_0^{n-1}) = 2kg'(t_n) \\ \Delta_{+t}\Delta_{-t}(\phi_N^n + \phi_{N+1}^n) + \lambda \Delta_{+x}(\phi_N^{n+1} - \phi_N^{n-1}) = 0 . \end{cases}$$

For each boundary condition three cases were run:

NOPER: No perturbation

INPER: Perturbation 0.001 in ϕ_j^1, $j = 0, 1, \ldots, N+1$

BOPER: Perturbation 0.001 in the right boundary condition.

In all cases the boundary function $g(t) = \sin t$ was used, which gives a discontinuity in the second derivatives of ϕ. Table 2.1 shows the mean-square error in the solution at $t = 4$.

	BC0		BC1		BC2	
	$h = 1/20$	$h = 1/40$	$h = 1/20$	$h = 1/40$	$h = 1/20$	$h = 1/40$
NOPER	$7.0e-5$	$2.1e-5$	$2.0e-4$	$5.1e-5$	$3.5e-2$	$1.8e-2$
INPER	$3.8e-3$	$3.9e-3$	$1.4e-2$	$2.6e-2$	$1.4e-1$	$2.2e-1$
BOPER	$6.0e-4$	$4.2e-4$	$4.0e-2$	$7.9e-2$	$3.5e+0$	$1.4e+1$

Table 2.1. Mean-square error in ϕ at $t = 4$.

The perturbations have a disastrous effect for BC2, in particular when the perturbation occurs in the boundary condition. BC1 is also more sensitive to perturbations than BC0, as expected. When no perturbation is introduced, BC2 still gives a poor accuracy, and the convergence rate is clearly only of first order.

We have not included any forcing function in the discussion above. When deriving error-estimates for the approximation ϕ_j^n, such a forcing function F_j^n represents the truncation error, and is necessarily present in the difference scheme for the error $\phi_j^n - \phi(x_j, t_n)$. The grid function F_j^n depends on $\phi(x,t)$, and is small only if ϕ is sufficiently smooth. The results above show that if this is not the case, the boundary condition BC1 is more forgiving than BC2.

For multi-dimensional problems it is more difficult to keep the solution smooth enough, in particular when the numerical method requires extra numerical boundary conditions. The conclusion from this section is therefore that derivative bundary conditions should be avoided for hyperbolic problems. In the next section we shall show how accurate and well-posed conditions still can be derived.

3. First order systems

In this section we consider general first order hyperbolic systems. We shall discuss the implementation of the boundary conditions and how to provide accurate data at the boundary. If the system has variable coefficients or is non-linear, then the coefficients are frozen outside the computational domain; usually the values at infinity are used. It is important to distinguish between this procedure, and the method of using values from the state at infinity for the variables at the computational boundary. In the first case, the solution is still allowed to vary outside the computational domain, but it satisfies a simpler differential equation. In this way the form of the solution can be explicitly derived, such that boundary conditions can be obtained. As in Section 2, we shall consider the case where the computational domain is infinite in the y-direction but has a boundary at $x = 0$. The right half-plane is the domain for computation, the solution in the left half-plane is supposed to have a simpler structure, such that this part can be eliminated from the computation. (In practice, there is of course another computational boundary for some positive x, as well as in both y-directions.) In order to derive conditions at $x = 0$, we therefore consider the problem

$$
(3.1) \qquad \begin{cases} \text{(a)} & U_t + AU_x + BU_y = 0\,, \quad -\infty < x \le 0,\ -\infty < y < \infty,\ 0 \le t \\ \text{(b)} & \sup_{x,y} |U(x,y,t)| < \infty\,, \quad 0 \le t \\ \text{(c)} & U(x,y,0) = f(x,y)\,, \quad -\infty < x \le 0,\ -\infty < y < \infty\,. \end{cases}
$$

In [4] we have treated this problem, and we briefly summarize the results here. It is a generalization of the absorbing boundary conditions derived in [1].

Since the system is hyperbolic, the matrix A can be diagonalized, and it is assumed that this has already been done here, such that

$$A = \mathrm{diag}(a_1, a_2, \ldots, a_{l+m})$$

where

$$\begin{aligned} a_j &> 0\,, \qquad j = 1,2,\ldots,l \\ a_{j+l} &< 0\,, \qquad j = 1,2,\ldots,m\,. \end{aligned}$$

The system (3.1a) is Laplace-transformed in time and Fourier-transformed in the y-direction, s and ω being the dual variables. For the transformed vector $\hat{U}$ we get the equation

$$\hat{U}_x(x,\omega,s) = -sQ(\xi)\hat{U}(x,\omega,s) + A^{-1}\,\tilde{f}(x,\omega)\,,$$

where

$$Q(\xi) = A^{-1}(I + \xi B)\,, \qquad \xi = i\omega/s\,,$$

and where $\tilde{f}(x,\omega)$ is the Fourier-transformed initial function. For Re $s > 0$, the matrix $Q(\xi)$ can be transformed to block-diagonal form

$$T^{-1}(\xi)Q(\xi)T(\xi) = \begin{bmatrix} Q^I(\xi) & 0 \\ 0 & Q^{II}(\xi) \end{bmatrix},$$

where, corresponding to the eigenvalues of A, $Q^I(\xi)$, $Q^{II}(\xi)$ are $(l \times l)$- and $(m \times m)$-matrices respectively. The condition (3.1b) implies the condition

$$[T^{-1}(\xi)\hat{U}(0,\omega,s)]^I = -\int_0^\infty e^{sQ^I\sigma}[T^{-1}(\xi)A^{-1}\,\tilde{f}(\sigma,\omega)]^I\,d\sigma \tag{3.2}$$

where $[V]^I$ indicates the upper l elements of the vector V. This is the exact boundary condition for the problem defined in the domain $x \geq 0$. For $f \equiv 0$, it is the completely absorbing boundary condition by Engquist and Majda. In order to get local boundary conditions in physical space, some approximations must be made.

Let κ_j, $j = 1,2,\ldots,l$ be the eigenvalues of $-sQ^I(\xi)$, and assume that $Q^I(\xi)$ can be transformed to diagonal form. Assuming that this transformation is included in the matrix $T(\xi)$ above, the equation (3.2) can be written in the form

$$[T^{-1}(\xi)]_j\hat{U}(0,\omega,s) = -[T^{-1}(\xi)A^{-1}]_j\int_0^\infty e^{-\kappa_j\sigma}\,\tilde{f}(\sigma,\omega)\,d\sigma\,, \quad j = 1,2,\ldots,l \tag{3.3}$$

where $[A]_j$ denotes the j-th row of the matrix A. If $|\xi|$ is small, we use the expansions

$$\begin{cases} \text{(a)} & T^{-1}(\xi) = I + R\xi + S\xi^2 + O(|\xi|^3) \\ \text{(b)} & \kappa_j = -s(a_j^{-1} + \beta_j\xi + O(|\xi|^2))\,, \qquad j = 1,2,\ldots,l \end{cases} \tag{3.4}$$

in (3.3). If ξ-terms of order one and higher are disregarded, we get after transforming back to physical space

$$U^{(j)}(0,y,t) = f^{(j)}(-a_j t, y)\,, \qquad j = 1,2,\ldots,l\,. \tag{3.5}$$

This condition is obtained directly from (3.1a) by letting $B = 0$, and then solving the one-dimensional system exactly. If the ξ-terms of first order are kept, we get after a straightforward calculation

$$U^{(j)}(0,y,t) + \int_0^t R_j U_y(0,y,\tau)\,d\tau = g(y,t)\,, \tag{3.6}$$

where

$$g(y,t) = f^{(j)}(-a_j t, y - \beta_j a_j t) + a_j [RA^{-1}]_j \int_0^t f_y(-a_j\tau, y - \beta_j a_j \tau)\,d\tau\,, \qquad j = 1,2,\ldots,l\,.$$

These are the boundary conditions for the problem

$$\begin{cases} U_t + AU_x + BU_y = 0\,, & 0 \le x < \infty,\ -\infty < y < \infty,\ 0 \le t \\ \sup_{x,y} |U(x,y,t)| < \infty\,, & 0 \le t \\ U(x,y,0) = f(x,y)\,, & 0 \le x < \infty,\ -\infty < y < \infty. \end{cases} \tag{3.7}$$

There is no proof of well-posedness for general systems, but we assume that (3.7), (3.6) is well-posed such that there is an estimate

$$\|U(\cdot,\cdot,t)\|^2 + \int_0^t \|U(0,\cdot,\tau)\|^2\,d\tau \le C\left(\|f(\cdot,\cdot)\|^2 + \int_0^t \|g(\cdot,\tau)\|^2\,d\tau\right). \tag{3.8}$$

Here $\|U(\cdot,\cdot,t)\|$ is the L_2-norm over the right half-plane, and $\|U(x,\cdot,t)\|$ is the L_2-norm over $\{y/-\infty < y < \infty\}$.

At this point we make a remark concerning the theory for well-posedness. The Kreiss theory was developed for first order systems with boundary conditions of the type

$$S_0 U(0,y,t) = g(y,t)$$

where S_0 is a constant rectangular matrix. In transformed space the boundary condition can be written as

$$\hat{B}^I(\omega,s)\hat{V}^I(0,\omega,s) = \hat{B}^{II}(\omega,s)\hat{V}^{II}(0,\omega,s) + \hat{g}(\omega,s)\,, \qquad \hat{V} = T^{-1}\hat{U}\,,$$

and the condition for well-posedness is

$$\mathrm{Det}\big(\hat{B}^I(\omega,s)\big) \neq 0\,, \qquad \mathrm{Im}\,\omega = 0\,, \quad \mathrm{Re}\,s \ge 0\,. \tag{3.9}$$

For $s \neq 0$, it is clear from the construction above, that $\hat{B}^I$ is a function of the single variable $\xi = i\omega/s$. For $\omega = 0$, $\hat{B}^I$ is a constant matrix, consisting of the first l columns of S_0, accordingly, the condition for well-posedness is independent of s. It follows from these arguments that it is sufficient to consider the domain $|\omega| + |s| = 1$ when verifying the Kreiss condition.

If, on the other hand, derivatives occur in the boundary conditions, then $\hat{B}^I$ may depend on s even for $\omega = 0$, and the point $\omega = s = 0$ must be included.

If the conditions (3.6) are differentiated with respect to t, we get

$$U_t^{(j)}(0,y,t) + R_j U_y(0,y,t) = g_t(y,t)\,, \qquad j = 1,2,\ldots,l\,. \tag{3.10}$$

These conditions are less suitable for computations. We have

Lemma 3.1. *The problem (3.7), (3.10) is at least weakly ill-posed.*

Proof. For $\omega = 0$, the condition (3.9) is

$$\mathrm{Det}(sI) \neq 0\,, \qquad \mathrm{Re}\, s \geq 0$$

which is obviously violated at $s = 0$.

As for the wave equation, we conclude that the condition (3.6) is a better basis for an approximation than the condition (3.10). In [4] an experiment was carried out, clearly demonstrating this. Note that the condition (3.6) is no more difficult to implement than the condition (3.10). The integral is substituted by a sum, and for each y-value one new term is added for each times-step.

In many applications there is a source outside the computational domain, which is driving the solution. Sometimes this situation can be modeled as an initial value problem where the initial function $f(x, y)$ is known everywhere. However, in order to avoid the approximations that are necessary in the general case, a better method may be to prescribe the correct data directly at the boundary.

Assume that the solution consists of two parts U_0, U_1, where U_0 is known. A typical case is where U_0 is a plane wave produced by an outer source. In the computational domain there is some interaction which causes the generation of U_1, and it is assumed that this part of the solution can be considered as a wave that passes out through the boundary. In such a case, the initial data occurring in (3.5) and (3.6) are substituted by the known forced solution U_0. The conditions (3.5) and (3.6) for $U = U_0 + U_1$ takes the form

$$U^{(j)}(0, y, t) = U_0^{(j)}(0, y, t)\,, \qquad j = 1, 2, \ldots, l \tag{3.11}$$

$$U^{(j)}(0, y, t) + \int_0^t R_j U_y(0, y, \tau)\, d\tau = U_0^{(j)}(0, y, t) + \int_0^t R_j[(U_0)_y](0, y, \tau)\, d\tau\,, \quad j = 1, 2, \ldots, l\,. \tag{3.12}$$

Consider next the wave equation (2.1). From the discussion in Section 2 it is clear that there are certain advantages with using the corresponding first order system as a basis for the approximation. With

$$V = \begin{bmatrix} \tilde{u} \\ \tilde{v} \\ \tilde{w} \end{bmatrix} = \begin{bmatrix} -\phi_t \\ \phi_x \\ \phi_y \end{bmatrix}\,,$$

we get

$$V_t + \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} V_x + \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} V_y = 0\,. \tag{3.13}$$

The coefficient matrix multiplying V_x is singular, hence the technique used above does not apply directly. We modify the system by subtracting a term ϵV_x, $\epsilon > 0$, and after deriving the boundary conditions we let $\epsilon \to 0$. With the new variables

$$u = \frac{\tilde{u} + \tilde{v}}{\sqrt{2}}\,, \quad v = \frac{\tilde{u} - \tilde{v}}{\sqrt{2}}\,, \quad w = \tilde{w}\,,$$

we get the system

$$U_t + AU_x + BU_y = 0 \tag{3.14}$$

where

$$A = \begin{bmatrix} 1-\epsilon & 0 & 0 \\ 0 & -1-\epsilon & 0 \\ 0 & 0 & -\epsilon \end{bmatrix}, \qquad B = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

The matrix R and the eigenvalues κ_j in (3.4) are

$$R = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & \epsilon \\ 0 & 0 & -\epsilon \\ 1-\epsilon & 1+\epsilon & 0 \end{bmatrix},$$

$$\kappa_1 = -s\left(\tfrac{1}{1-\epsilon} - \tfrac{\xi^2}{2} + O(|\xi|^4)\right)$$

$$\kappa_2 = -s\left(-\tfrac{1}{1+\epsilon} + \tfrac{\xi^2}{2} + O(|\xi|^4)\right)$$

$$\kappa_3 = s/\epsilon\,.$$

There is only one eigenvalue κ_1 with $\mathrm{Re}\ \kappa < 0$ for $\mathrm{Re}\ s > 0$, hence the boundary condition is determined by the first row of R. The condition (3.12) becomes

$$v(0,y,t) + \frac{\epsilon}{\sqrt{2}} \int_0^t w_y(0,y,\tau)\,d\tau = v\big(-(1-\epsilon)t, y, 0\big) - \frac{1-\epsilon}{\sqrt{2}} \int_0^t w_y\big(-(1-\epsilon)\tau, y, 0\big)\,d\tau\,. \tag{3.15}$$

Since the matrix row $[RA^{-1}]_1$ in (3.6) is well defined even for $\epsilon = 0$, the limit of (3.15) as $\epsilon \to 0$ is also well defined. In the original variables the condition becomes

$$[\tilde{u} + \tilde{v}](0,y,t) = [\tilde{u} + \tilde{v}](-t,y,0) - \int_0^t \tilde{w}_y(-\tau,y,0)\,d\tau\,. \tag{3.16}$$

If the right hand side is considered as given data, the condition (3.16) is trivially well-posed. We note that for zero initial data, there is no difference between the first and second order conditions.

A third order condition would be obtained by including the third term in the expansion (3.4a),

$$T^{-1}(\xi) \approx I + R\xi + S\xi^2\,, \qquad S = -\frac{1-\epsilon^2}{4} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

Considering zero initial data, we get from the transformed differential equation (3.14)

$$\xi(\hat{u} + \hat{v}) = \sqrt{2}\left(\frac{\epsilon}{s}\hat{w}_x - \hat{w}\right),$$

and by inserting this into the second row of S, we get for $\epsilon = 0$,

$$\hat{u} + \frac{\xi}{2\sqrt{2}}\hat{w} = 0\,. \tag{3.17}$$

In physical space this condition is for the original variables

$$[\tilde{u}+\tilde{v}](0,y,t)+\frac{1}{2}\int_0^t \tilde{w}_y(0,y,\tau)\,d\tau = g(y,t)\,, \tag{3.18}$$

where we have included the possibility of giving non-zero boundary data. By differentiating with respect to t and going back to the wave-function ϕ in (2.1), we obtain

$$-\phi_{tt}+\phi_{xt}+\tfrac{1}{2}\phi_{yy} = g_t(y,t)\,, \qquad x=0\,, \tag{3.19}$$

which we recognize as the condition (2.9) with $g=-g_t$.

The well-posedness of the first and second order conditions is trivial. For the third order one we have

Theorem 3.1. *The wave equation formulated as a first order system (3.13) is well-posed with the boundary condition (3.18).*

Proof. The first column of the matrix T which transforms $\hat{Q}(\xi)$ to diagonal form is

$$[T(\xi)]^{(1)} = [1-\kappa_1/s\,,\ 1+\kappa_1/s\,,\ -\sqrt{2}(1-\kappa_1^2/s^2)/\xi]^T\,,$$

Referring to Section 4 of [4], we obtain the condition for well-posedness from (3.17) as

$$1-\frac{\kappa_1}{s}-\frac{1}{2}\left(1-\frac{\kappa_1^2}{s^2}\right)\neq 0\,,$$
$$\kappa_1 = \pm s\sqrt{1-\xi^2}\,.$$

The sign of κ_1 is taken such that $\mathrm{Re}\,\kappa_1<0$ for $\mathrm{Re}\,s>0$. (Note that it is not sufficient to consider small values of $|\xi|$ here.) The critical points are therefore given by

$$1\mp\sqrt{1-\xi^2}=0 \tag{3.20}$$

and

$$1-\frac{1}{2}\left(1\pm\sqrt{1-\xi^2}\right)=0\,. \tag{3.21}$$

The condition (3.20) implies $\xi=0$, which is the one-dimensional case known to be well-posed. The condition (3.21) implies

$$\pm\sqrt{1-\xi^2}=1\,,$$

which again leads to the one-dimensional case $\xi=0$, and the theorem is proven.

If one prefers to use the scalar wave equation, then the condition (3.18) takes the form

$$-\phi_t(0,y,t)+\phi_x(0,y,t)+\tfrac{1}{2}\int_0^t \phi_y(0,y,\tau)\,d\tau = g(y,t)$$

which is the integrated form of (3.19). In one space-dimension it is equivalent to the first order condition (2.4) denoted by BC1 in Section 2; the condition (3.19) corresponds to BC2. Table 2.1

shows that the integrated version is preferable. The numerical experiments prescribed in [4] for two-dimensional problems confirms this conclusion.

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